KINETIC MODELLING OF ETHANOL PRODUCTION FROM OIL PALM TRUNK SAP DURING FERMENTATION

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We hereby declare that we have checked this thesis and in our opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Master of Science.

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I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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ABSTRAK

Penyimpanan bahan api fosil di seluruh dunia yang terhad dan impaknya yang buruk terhadap alam sekitar membawa kepada penyelidikan terkini ke arah penggunaan biomas dalam penghasilan biofuel. Malaysia kaya dengan sumber biomas. Batang kelapa sawit (OPT) adalah sumber biomas untuk meghasilkan bioethanol. Fermentasi adalah proses terpenting dalam penukaran biomas kepada etanol. Model kinetik yang sesuai mampu meningkatkan kecekapan dan proses pengoptimuman penapaian etanol menggunakan sap OPT. Kaedah teoritikal lebih efisien dan memerlukan kos pelaburan yang rendah, tetapi kaedah ini sukar untuk disahkan. Beberapa model kinetik telah dicadangkan tetapi tiada model yang mengambil kira faktor-faktor penting seperti batasan substrat, perencat substrat, penghambatan produk, dan kematian sel secara serentak pada suhu berbeza untuk menghasilkan etanol dari penapaian sap OPT. Kami memanjangkan dan memperbaiki model matematik terkini untuk meneroka kesan suhu, kepekatan sel terawal dan kadar kematian sel pada proses penapaian. Beberapa parameter kinetik digunakan untuk menggambarkan fenomena ini. Satu set persamaan pembezaan biasa digunakan untuk memodelkan profil gula, sel dan etanol untuk penapaian sap OPT dan persamaan telah diselesaikan oleh kaedah Runge-Kutta untuk ke-4. Terdapat dua set hasil simulasi yang dibentangkan dalam kajian ini untuk Model I dan II. Model I adalah model mudah yang memanjangkan model Oliviera, di mana kami mengkaji kesan kadar kematian sel. Model II lebih komprehensif dan lebih baik daripada Model I, kerana ia mempunyai hubungan Leudeking-Piret, model Phisalaphong dan juga Model I. Sesetengah ciri-ciri penting dikenalpasti kedua-dua model. Apabila suhu meningkat, kadar pertumbuhan sel khusus maksimum menurun bagi kedua-dua model. Dari hasilnya, Suhu yang sesuai untuk pengeluaran etanol dari penapaian sap OPT ialah 30°C. Kadar penggunaan gula dan pengeluaran etanol sepanjang proses penapaian bergantung pada kepekatan sel awal. Dengan kepekatan sel awal yang rendah, kadar penukaran meningkat secara beransur-ansur tetapi untuk kepekatan sel awal yang tinggi, penukaran gula ke etanol meningkat dengan ketara dan berkurangan selepas tempoh yang singkat disebabkan oleh akses etanol, yang mungkin menghalang pertumbuhan sel. Pertimbangan gabungan batasan dan perencatan substrat, penghambatan produk dan kadar kematian sel meningkatkan ketepatan model I dengan cara rRMSE. Pemerhatian serupa ditemui untuk model II apabila faktor-faktor yang dipertimbangkan adalah had dan penyekatan substrat, pertumbuhan dan pembentukan produk yang berkaitan dengan pertumbuhan, penghambatan produk dan kematian sel. Pendekatan ini membolehkan kita memperoleh keupayaan ramalan yang lebih baik dengan itu meningkatkan pemahaman kita terhadap model matematik penapaian sap OPT.

ABSTRACT

The worldwide limited storage of fossil fuel and its bad impact on environment lead to the recent research towards biomass for biofuel. Malaysia is rich with plenty of biomass resources. Oil palm trunk (OPT) is a promising biomass source for bioethanol production. Fermentation is an essential process of biomass to ethanol conversion. An appropriate kinetic model will be a powerful tool to increase the efficiency and process optimization for ethanol fermentation using the OPT sap. The theoretical methods are more efficient and require low investment, but it is challenging to validate. A number of kinetic models have been proposed but none of these models observed the effect of most essential factors such as substrate limitation, substrate inhibition, product inhibition, and cell death simultaneously on temperature to produce ethanol from the OPT sap fermentation. We extended and improved the current mathematical model to explore the effect of temperature, initial cell concentration and cell death rate on the fermentation process. Several kinetic parameters were used to describe this phenomenon. A set of ordinary differential equations were used to modelled the profiles of sugar, cell and ethanol for the fermentation of OPT sap and the equations were solved by the 4th order Runge-Kutta method. There are two sets of simulation results presented in this study for Model I and II. Model I is a simple model which extends Oliviera's model, where we studied the effect of cell death rate. Model II is more comprehensive and better than Model I, because it consists Leudeking-Piret relationship, Phisalaphong model and also Model I. Some significant characteristics are apprehended both of the models. As the temperature increased, the maximum specific cell growth rate decreased for both of the models. From the results, the suitable temperature for ethanol production from the OPT sap fermentation is 30°C. The rate of sugar utilisation and ethanol production throughout fermentation process depend on the initial cell concentration. With the low initial cell concentration, the conversion rate was increased gradually but for the high initial cell concentration, sugar conversion to ethanol was augmented sharply and depleted after the short duration due to access of the ethanol, which might inhibit the cell growth. The combined consideration of the substrate limitation and inhibition, growth and non-growth associated product formation, product inhibition and cell death rate increased the accuracy of the Model II by means of rRMSE. This approach has enabled us to obtained a better predictive capabilities hence increasing our understanding of the mathematical model of the OPT sap fermentation.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF SYMBOLS

a	growth associated specific productivity coefficient
b	Non-growth associated specific productivity coefficient
c	Coefficient of cell maintenance
$f\left(x_i\right)$	Calculated data
K_{CM}	Maintenance constant
K_d	Cell death rate
K_i	Substrate inhibition coefficient/ Inhibition parameter for sugar
K_S	Saturation constant of substrate/ Substrate inhibition constant
$K_{in,S}$	Substrate inhibition constant
$K_{li,S}$	Substrate limitation constant
$K_{li,O2}$	Dissolved oxygen limitation constant
K_P	Product inhibition constant
K_{SP}	Saturation constant for ethanol production
K_{SS}	Substrate inhibition term for cell growth
K_{SSP}	Substrate inhibition term for ethanol production
n	Ethanol toxic power
O_2	Dissolved oxygen concentration
P	Ethanol production
P_m	Ethanol inhibition term for cell growth
P'_M	Ethanol inhibition term for ethanol production
P^*	Critical concentration of product
r	Reaction rate
$Y'_{X/S}$, $Y_{X/S}$	Yield coefficient for the cell on substrate
$Y'_{P/S}$, $Y_{P/S}$	Yield coefficient for the ethanol on substrate
y_i	Experimental data
α	Model parameter
μ	Specific growth rate

$\hat{\mu}$	Maximum specific growth rate
ν	Specific production rate

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